

Chlorotrifluoroethylene
79-38-9 | DTXSID3026485

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.84 | 0.55 | 0.85 | 0.53 | 0.83 | 0.64 |

Model Results

Predicted value: 14.9

Global applicability domain: Inside

Local applicability domain index: 3.93e-01

Confidence level: 6.61e-01

Nearest Neighbors from the Training Set

| | | |
|--|--|---|
| <div>Image not found</div> <div>Dichlorodifluoromethane</div> <div>Measured: 6.17</div> <div>Predicted: 9.03</div> | <div>Image not found</div> <div>1,1,2-Trichloro-1,2,2-trifluoroethane</div> <div>Measured: 50.1</div> <div>Predicted: 37.1</div> | <div>Image not found</div> <div>Isoprene</div> <div>Measured: 20.0</div> <div>Predicted: 15.6</div> |
| <div>Image not found</div> <div>4-Nitrophenol</div> <div>Measured: 5.13</div> <div>Predicted: 3.67</div> | <div>Image not found</div> <div>3-Nitrophenol</div> <div>Measured: 25.1</div> <div>Predicted: 3.67</div> | |